

Tris(ethylenediamine- κ^2N,N')cobalt(III) aquatrakis(oxalato- κ^2O^1,O^2)indate(III)

Zhe Zhang, Fuxiang Wang and Shuangquan Liao*

Department of Materials and Chemical Engineering, Ministry of Education Key Laboratory of Application Technology of Hainan Superior Resources Chemical Materials, Hainan University, Haikou 570228, Hainan Province, People's Republic of China

Correspondence e-mail: shqliao@126.com

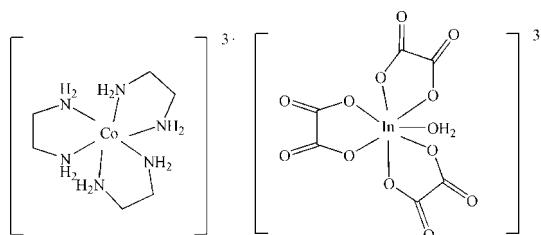
Received 26 November 2011; accepted 13 December 2011

Key indicators: single-crystal X-ray study; $T = 293\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$; R factor = 0.048; wR factor = 0.119; data-to-parameter ratio = 16.6.

In the cation of the title compound, $[\text{Co}(\text{C}_2\text{H}_8\text{N}_2)_3][\text{In}(\text{C}_2\text{O}_4)_3(\text{H}_2\text{O})]$, the Co^{III} atom is coordinated by six N atoms from three ethylenediamine molecules. The $\text{Co}^{III}-\text{N}$ bond lengths lie in the range 1.956 (4)–1.986 (4) Å. In the anion, the In^{III} atom is seven-coordinated by six O atoms from three oxalate ligands and by a water molecule. The cations and anions are linked by extensive $\text{O}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a supermolecular network.

Related literature

For metal phosphates and germanates templated by metal complexes, see: Du *et al.* (2004); Pan *et al.* (2005, 2008); Wang *et al.* (2003a,b,c). For coordination polymers templated by metal complexes, see: Pan *et al.* (2010a,b, 2011), Tong & Pan (2011).



Experimental

Crystal data

$[\text{Co}(\text{C}_2\text{H}_8\text{N}_2)_3][\text{In}(\text{C}_2\text{O}_4)_3(\text{H}_2\text{O})]$

$M_r = 636.14$

Triclinic, $P\bar{1}$

$a = 7.5161$ (15) Å

$b = 10.921$ (2) Å

$c = 14.450$ (3) Å

$\alpha = 79.43$ (3)°

$\beta = 80.13$ (3)°

$\gamma = 71.25$ (3)°

$V = 1096.1$ (4) Å³

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 1.89\text{ mm}^{-1}$

$T = 293\text{ K}$

$0.3 \times 0.2 \times 0.18\text{ mm}$

Data collection

Rigaku R-AXIS RAPID-S

diffractometer

Absorption correction: multi-scan
(*CrystalClear*; Rigaku/MSC,
2002)

$T_{\min} = 0.6$, $T_{\max} = 0.8$

11056 measured reflections

4988 independent reflections

4360 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.056$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.119$

$S = 1.10$

4988 reflections

300 parameters

Only H-atom displacement para-meters refined

$\Delta\rho_{\max} = 1.32\text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.91\text{ e \AA}^{-3}$

Table 1
Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O13—H13A···O12 ⁱ	0.91	1.79	2.620 (5)	150
O13—H13B···O6 ⁱⁱ	0.86	1.84	2.629 (4)	152
N1—H1A···O11 ⁱⁱⁱ	0.90	2.17	3.064 (5)	171
N1—H1B···O8 ^{iv}	0.90	2.14	2.972 (5)	153
N2—H2A···O7 ^v	0.90	2.10	2.935 (5)	155
N2—H2B···O10 ^{vi}	0.90	2.01	2.838 (5)	152
N3—H3A···O7 ^v	0.90	2.34	3.142 (5)	149
N3—H3A···O3 ^v	0.90	2.37	3.063 (5)	134
N3—H3B···O6 ^{iv}	0.90	2.06	2.878 (5)	151
N4—H4A···O1 ⁱⁱⁱ	0.90	2.26	3.114 (5)	159
N4—H4A···O2 ⁱⁱⁱ	0.90	2.49	3.103 (5)	126
N4—H4B···O2	0.90	2.04	2.924 (6)	168
N5—H5A···O8 ^v	0.90	2.09	2.962 (5)	163
N5—H5B···O4	0.90	2.14	2.912 (5)	143
N5—H5B···O2	0.90	2.40	3.099 (5)	135
N6—H6A···O11 ⁱⁱⁱ	0.90	2.27	3.040 (5)	143
N6—H6A···O1 ⁱⁱⁱ	0.90	2.49	3.279 (5)	147
N6—H6B···O10 ^{vi}	0.90	2.31	3.105 (5)	147

Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $x + 1, y, z$; (iii) $-x, -y + 1, -z + 2$; (iv) $-x, -y, -z + 2$; (v) $-x + 1, -y, -z + 2$; (vi) $x, y, z + 1$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystEngComm* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Foundation of Hainan University (No. hd09xm69) and the University Scientific Research Foundation of the Education Committee of Hainan Province (No. HJKL2009–16).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2490).

References

- Du, Y., Yu, J. H. & Xu, R. R. (2004). *J. Solid State Chem.* **177**, 2032–2037.
- Pan, Q. H., Cheng, Q. & Bu, X.-H. (2010b). *CrystEngComm*, **12**, 4198–4204.
- Pan, Q. H., Cheng, Q. & Bu, X.-H. (2011). *Chem. J. Chin. Univ.* **32**, 527–531.
- Pan, Q. H., Li, J. Y. & Bu, X.-H. (2010a). *Microporous Mesoporous Mater.* **132**, 453–457.
- Pan, Q. H., Yu, J. H. & Xu, R. R. (2005). *Chem. J. Chin. Univ.* **26**, 2199–2202.
- Pan, Q. H., Yu, J. H. & Xu, R. R. (2008). *Chem. Mater.* **20**, 370–372.
- Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.

metal-organic compounds

- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
Tong, J. & Pan, Q. (2011). *Acta Cryst. E* **67**, m579–m580.
Wang, Y., Yu, J. H. & Xu, R. R. (2003a). *J. Solid State Chem.* **170**, 176–3037.
Wang, Y., Yu, J. H. & Xu, R. R. (2003b). *Angew. Chem. Int. Ed.* **42**, 4089–4092.
Wang, Y., Yu, J. H. & Xu, R. R. (2003c). *Chem. Eur. J.* **9**, 5048–5055.

supplementary materials

Acta Cryst. (2012). E68, m65-m66 [doi:10.1107/S1600536811053736]

Tris(ethylenediamine- κ^2N,N')cobalt(III) aquatris(oxalato- κ^2O^1,O^2)indate(III)

Z. Zhang, F. Wang and S. Liao

Comment

Currently, more attention has been paid to employ chiral metal complexes as template, for its wide of shapes, charges and particularly chirality. Up to now, series of metal phosphates and germanates with interesting stuctures have been prepared by using such chiral metal complexes as the template (Wang *et al.*, 2003a; Pan *et al.* 2005, 2008; Du *et al.* 2004). And a new concept of chirality transfer of the metal complex into the inorganic host framework has been demonstrated by Yu *et al.* (Wang *et al.*, 2003b,c). Recently, Pan *et al.* introduced it into the system coordination polymers, a series of metal oxalates were obtained using metal complex cations as template (Pan *et al.*, 2010a,b, 2011). More recently, they reported $[Co(C_2H_8N_2)_3]^{3+}[In(C_2O_4)_2(CH_2O_2)_2]^{3-} \cdot 2H_2O$, a formate oxalate mixed coordinated complex (Tong & Pan 2011). In this paper, we present a new complex $[Co(C_2H_8N_2)_3]^{3+}[In(C_2O_4)_3(H_2O)]^{3-}$. As shown in Fig. 1, the crystal structure of (I) consists of a discrete $[In(C_2O_4)_3(H_2O)]^{3-}$ anions and $[Co(en)_3]^{3+}$ cations. The In^{III} ions was seven coordinated and surrounded by three different chelting oxalate and a coordinated water molecule. And the Co^{III} atom in the cation was connected six N atoms from three different chelting ethylenediamine in a distorted octahedral geometry. The cations and the anions were connected each other through hydrogen bonds to giving a supermolecule entity.

Experimental

In a typical synthesis, a mixture of $In(NO_3)_3 \cdot 5H_2O$ (1 mmol), $Co(en)_3Cl_3$ (0.14 mmol), $K_2C_2O_4 \cdot H_2O$ (2 mmol) and H_2O (10 ml), was added to a 20 ml Teflon-lined reactor under autogenous pressure at 120 °C for 4 days.

Refinement

All H atoms were positioned geometrically ($C-H = 0.97 \text{ \AA}$, $N-H = 0.90 \text{ \AA}$ and $O-H = 0.85 \text{ \AA}$) and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(\text{parent atom})$.

Figures

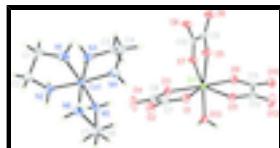


Fig. 1. A view of the structure of complex. Ellipsoids are drawn at the 30% probability level.

supplementary materials

Tris(ethylenediamine- κ^2N,N')cobalt(III) aquatris(oxalato- κ^2O^1,O^2)indate(III)

Crystal data

[Co(C ₂ H ₈ N ₂) ₃][In(C ₂ O ₄) ₃ (H ₂ O)]	Z = 2
M _r = 636.14	F(000) = 640
Triclinic, P <bar{1}< bar=""></bar{1}<>	D _x = 1.927 Mg m ⁻³
a = 7.5161 (15) Å	Mo K α radiation, λ = 0.71073 Å
b = 10.921 (2) Å	Cell parameters from 10592 reflections
c = 14.450 (3) Å	θ = 3.0–27.5°
α = 79.43 (3)°	μ = 1.89 mm ⁻¹
β = 80.13 (3)°	T = 293 K
γ = 71.25 (3)°	Block, yellow
V = 1096.1 (4) Å ³	0.3 × 0.2 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer	4988 independent reflections
Radiation source: fine-focus sealed tube graphite	4360 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.056$
Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku/MSC, 2002)	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.0^\circ$
$T_{\text{min}} = 0.6$, $T_{\text{max}} = 0.8$	$h = -9 \rightarrow 9$
11056 measured reflections	$k = -14 \rightarrow 14$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.048$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.119$	Only H-atom displacement parameters refined
$S = 1.10$	$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2 + 0.7829P]$
4988 reflections	where $P = (F_o^2 + 2F_c^2)/3$
300 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 1.32 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.91 \text{ e \AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations

between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
In1	0.41280 (4)	0.27178 (3)	0.70832 (2)	0.02767 (11)
Co1	0.13688 (7)	0.26192 (5)	1.23880 (4)	0.02715 (15)
O1	0.2854 (5)	0.4022 (3)	0.8190 (2)	0.0379 (7)
O2	0.2698 (5)	0.4142 (3)	0.9718 (2)	0.0490 (9)
O3	0.5453 (5)	0.1704 (3)	0.8361 (2)	0.0402 (8)
O4	0.5603 (6)	0.1847 (4)	0.9864 (3)	0.0681 (12)
O5	0.1303 (4)	0.2508 (3)	0.7207 (3)	0.0400 (8)
O6	-0.0236 (4)	0.1146 (3)	0.7043 (3)	0.0480 (9)
O7	0.4574 (4)	0.0573 (3)	0.7116 (2)	0.0386 (7)
O8	0.2982 (5)	-0.0880 (3)	0.7345 (3)	0.0517 (9)
O9	0.4602 (5)	0.2478 (3)	0.5559 (2)	0.0449 (8)
O10	0.4079 (6)	0.3539 (4)	0.4111 (2)	0.0564 (10)
O11	0.2819 (4)	0.4654 (3)	0.6321 (2)	0.0349 (7)
O12	0.2215 (6)	0.5763 (4)	0.4920 (3)	0.0660 (12)
O13	0.6771 (4)	0.3184 (3)	0.6787 (2)	0.0382 (7)
H13A	0.690 (3)	0.380 (4)	0.628 (3)	0.080*
H13B	0.792 (5)	0.272 (2)	0.686 (3)	0.080*
N1	-0.1017 (6)	0.2554 (4)	1.3206 (3)	0.0410 (9)
H1A	-0.1676	0.3355	1.3353	0.080*
H1B	-0.1734	0.2288	1.2894	0.080*
N2	0.2587 (5)	0.1761 (4)	1.3530 (3)	0.0353 (8)
H2A	0.3232	0.0924	1.3464	0.080*
H2B	0.3414	0.2163	1.3607	0.080*
N3	0.1680 (5)	0.0943 (3)	1.1973 (3)	0.0362 (8)
H3A	0.2883	0.0433	1.2001	0.080*
H3B	0.0917	0.0534	1.2364	0.080*
N4	0.0045 (6)	0.3375 (4)	1.1268 (3)	0.0394 (9)
H4A	-0.1014	0.4015	1.1420	0.080*
H4B	0.0790	0.3727	1.0815	0.080*
N5	0.3809 (5)	0.2696 (3)	1.1686 (3)	0.0334 (8)
H5A	0.4736	0.2015	1.1922	0.080*
H5B	0.3818	0.2628	1.1074	0.080*
N6	0.1154 (5)	0.4369 (4)	1.2661 (3)	0.0376 (9)
H6A	-0.0062	0.4868	1.2690	0.080*
H6B	0.1564	0.4305	1.3223	0.080*
C1	-0.0561 (8)	0.1636 (5)	1.4084 (4)	0.0488 (12)
H1C	-0.0303	0.0745	1.3967	0.080*
H1D	-0.1620	0.1822	1.4579	0.080*

supplementary materials

C2	0.1141 (8)	0.1807 (5)	1.4380 (4)	0.0489 (12)
H2C	0.0817	0.2637	1.4616	0.080*
H2D	0.1630	0.1115	1.4881	0.080*
C3	0.1212 (8)	0.1146 (5)	1.0987 (4)	0.0470 (12)
H3C	0.0886	0.0404	1.0866	0.080*
H3D	0.2283	0.1253	1.0534	0.080*
C4	-0.0453 (8)	0.2366 (5)	1.0901 (4)	0.0490 (13)
H4C	-0.0684	0.2643	1.0244	0.080*
H4D	-0.1584	0.2208	1.1269	0.080*
C5	0.4190 (7)	0.3938 (4)	1.1746 (3)	0.0388 (10)
H5C	0.4919	0.4199	1.1165	0.080*
H5D	0.4909	0.3819	1.2270	0.080*
C6	0.2320 (7)	0.4966 (4)	1.1895 (3)	0.0384 (10)
H6C	0.2491	0.5728	1.2078	0.080*
H6D	0.1718	0.5228	1.1318	0.080*
C7	0.3368 (6)	0.3589 (4)	0.9016 (3)	0.0349 (10)
C8	0.4958 (7)	0.2256 (4)	0.9099 (3)	0.0396 (10)
C9	0.1204 (6)	0.1394 (4)	0.7148 (3)	0.0345 (10)
C10	0.3067 (6)	0.0259 (4)	0.7209 (3)	0.0347 (10)
C11	0.3953 (7)	0.3486 (5)	0.4982 (3)	0.0392 (11)
C12	0.2895 (6)	0.4741 (4)	0.5431 (3)	0.0380 (10)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
In1	0.02796 (18)	0.02283 (16)	0.03195 (19)	-0.00503 (12)	-0.00555 (12)	-0.00598 (11)
Co1	0.0254 (3)	0.0220 (3)	0.0337 (3)	-0.0050 (2)	-0.0045 (2)	-0.0058 (2)
O1	0.0447 (19)	0.0308 (15)	0.0320 (17)	0.0010 (13)	-0.0064 (14)	-0.0096 (13)
O2	0.063 (2)	0.0385 (18)	0.0382 (19)	-0.0011 (16)	-0.0030 (16)	-0.0148 (15)
O3	0.049 (2)	0.0324 (16)	0.0285 (17)	0.0043 (14)	-0.0057 (14)	-0.0049 (13)
O4	0.084 (3)	0.064 (2)	0.035 (2)	0.017 (2)	-0.021 (2)	-0.0108 (17)
O5	0.0311 (16)	0.0246 (15)	0.064 (2)	-0.0069 (13)	-0.0073 (15)	-0.0074 (14)
O6	0.0311 (17)	0.0337 (17)	0.081 (3)	-0.0111 (14)	-0.0150 (17)	-0.0010 (16)
O7	0.0299 (16)	0.0235 (14)	0.064 (2)	-0.0061 (12)	-0.0103 (15)	-0.0092 (14)
O8	0.045 (2)	0.0237 (15)	0.090 (3)	-0.0096 (14)	-0.0235 (19)	-0.0037 (16)
O9	0.062 (2)	0.0368 (17)	0.0375 (19)	-0.0119 (16)	-0.0079 (16)	-0.0119 (14)
O10	0.088 (3)	0.064 (2)	0.0312 (19)	-0.037 (2)	-0.0131 (18)	-0.0094 (16)
O11	0.0371 (17)	0.0289 (15)	0.0360 (18)	-0.0072 (13)	-0.0048 (13)	-0.0018 (12)
O12	0.074 (3)	0.054 (2)	0.045 (2)	0.003 (2)	-0.001 (2)	0.0100 (18)
O13	0.0284 (16)	0.0433 (18)	0.0405 (19)	-0.0103 (14)	-0.0089 (14)	0.0036 (14)
N1	0.037 (2)	0.036 (2)	0.051 (3)	-0.0107 (17)	-0.0003 (18)	-0.0150 (18)
N2	0.034 (2)	0.038 (2)	0.032 (2)	-0.0093 (16)	-0.0043 (16)	-0.0031 (15)
N3	0.035 (2)	0.0281 (18)	0.045 (2)	-0.0071 (16)	-0.0074 (17)	-0.0065 (16)
N4	0.037 (2)	0.0297 (19)	0.051 (2)	-0.0055 (16)	-0.0143 (18)	-0.0031 (17)
N5	0.034 (2)	0.0295 (18)	0.034 (2)	-0.0058 (15)	-0.0048 (16)	-0.0040 (15)
N6	0.035 (2)	0.0336 (19)	0.045 (2)	-0.0090 (16)	-0.0006 (17)	-0.0140 (16)
C1	0.053 (3)	0.050 (3)	0.046 (3)	-0.025 (3)	0.013 (2)	-0.014 (2)
C2	0.053 (3)	0.058 (3)	0.037 (3)	-0.021 (3)	0.001 (2)	-0.009 (2)

C3	0.065 (3)	0.041 (3)	0.042 (3)	-0.020 (2)	-0.013 (2)	-0.011 (2)
C4	0.054 (3)	0.046 (3)	0.055 (3)	-0.016 (2)	-0.026 (3)	-0.006 (2)
C5	0.040 (3)	0.039 (2)	0.043 (3)	-0.018 (2)	-0.002 (2)	-0.010 (2)
C6	0.047 (3)	0.027 (2)	0.045 (3)	-0.016 (2)	-0.008 (2)	-0.0044 (19)
C7	0.035 (2)	0.028 (2)	0.040 (3)	-0.0077 (18)	-0.0037 (19)	-0.0062 (18)
C8	0.042 (3)	0.038 (2)	0.034 (3)	-0.006 (2)	-0.006 (2)	-0.0024 (19)
C9	0.029 (2)	0.029 (2)	0.045 (3)	-0.0074 (18)	-0.0074 (19)	-0.0020 (18)
C10	0.037 (2)	0.025 (2)	0.044 (3)	-0.0088 (18)	-0.014 (2)	-0.0025 (18)
C11	0.048 (3)	0.045 (3)	0.033 (3)	-0.024 (2)	-0.009 (2)	-0.005 (2)
C12	0.034 (2)	0.037 (2)	0.040 (3)	-0.0125 (19)	-0.002 (2)	0.0031 (19)

Geometric parameters (\AA , $^\circ$)

In1—O13	2.160 (3)	N2—H2B	0.9000
In1—O5	2.182 (3)	N3—C3	1.487 (6)
In1—O3	2.191 (3)	N3—H3A	0.9000
In1—O11	2.199 (3)	N3—H3B	0.9000
In1—O9	2.221 (3)	N4—C4	1.477 (6)
In1—O1	2.222 (3)	N4—H4A	0.9000
In1—O7	2.250 (3)	N4—H4B	0.9000
Co1—N4	1.956 (4)	N5—C5	1.494 (5)
Co1—N5	1.957 (4)	N5—H5A	0.9000
Co1—N2	1.959 (4)	N5—H5B	0.9000
Co1—N3	1.960 (4)	N6—C6	1.479 (6)
Co1—N6	1.972 (4)	N6—H6A	0.9000
Co1—N1	1.986 (4)	N6—H6B	0.9000
O1—C7	1.277 (5)	C1—C2	1.492 (7)
O2—C7	1.225 (5)	C1—H1C	0.9700
O3—C8	1.263 (5)	C1—H1D	0.9700
O4—C8	1.234 (6)	C2—H2C	0.9700
O5—C9	1.262 (5)	C2—H2D	0.9700
O6—C9	1.236 (5)	C3—C4	1.509 (7)
O7—C10	1.265 (5)	C3—H3C	0.9700
O8—C10	1.244 (5)	C3—H3D	0.9700
O9—C11	1.266 (6)	C4—H4C	0.9700
O10—C11	1.238 (6)	C4—H4D	0.9700
O11—C12	1.265 (5)	C5—C6	1.501 (6)
O12—C12	1.230 (6)	C5—H5C	0.9700
O13—H13A	0.9135	C5—H5D	0.9700
O13—H13B	0.8610	C6—H6C	0.9700
N1—C1	1.481 (7)	C6—H6D	0.9700
N1—H1A	0.9000	C7—C8	1.559 (6)
N1—H1B	0.9000	C9—C10	1.546 (6)
N2—C2	1.491 (6)	C11—C12	1.543 (7)
N2—H2A	0.9000		
O13—In1—O5	170.86 (11)	H4A—N4—H4B	108.1
O13—In1—O3	79.09 (12)	C5—N5—Co1	111.8 (3)
O5—In1—O3	109.59 (13)	C5—N5—H5A	109.3
O13—In1—O11	87.46 (12)	Co1—N5—H5A	109.3

supplementary materials

O5—In1—O11	83.75 (12)	C5—N5—H5B	109.3
O3—In1—O11	143.84 (12)	Co1—N5—H5B	109.3
O13—In1—O9	84.67 (13)	H5A—N5—H5B	107.9
O5—In1—O9	90.49 (13)	C6—N6—Co1	108.4 (3)
O3—In1—O9	136.66 (12)	C6—N6—H6A	110.0
O11—In1—O9	73.94 (12)	Co1—N6—H6A	110.0
O13—In1—O1	95.45 (12)	C6—N6—H6B	110.0
O5—In1—O1	84.56 (12)	Co1—N6—H6B	110.0
O3—In1—O1	73.95 (11)	H6A—N6—H6B	108.4
O11—In1—O1	74.14 (11)	N1—C1—C2	107.7 (4)
O9—In1—O1	148.04 (12)	N1—C1—H1C	110.2
O13—In1—O7	111.82 (12)	C2—C1—H1C	110.2
O5—In1—O7	74.38 (11)	N1—C1—H1D	110.2
O3—In1—O7	72.79 (12)	C2—C1—H1D	110.2
O11—In1—O7	142.94 (12)	H1C—C1—H1D	108.5
O9—In1—O7	76.66 (12)	N2—C2—C1	107.3 (4)
O1—In1—O7	131.28 (12)	N2—C2—H2C	110.2
N4—Co1—N5	92.52 (17)	C1—C2—H2C	110.2
N4—Co1—N2	175.52 (16)	N2—C2—H2D	110.2
N5—Co1—N2	90.62 (16)	C1—C2—H2D	110.2
N4—Co1—N3	84.54 (16)	H2C—C2—H2D	108.5
N5—Co1—N3	91.28 (16)	N3—C3—C4	106.4 (4)
N2—Co1—N3	92.20 (16)	N3—C3—H3C	110.5
N4—Co1—N6	91.28 (16)	C4—C3—H3C	110.5
N5—Co1—N6	84.23 (15)	N3—C3—H3D	110.5
N2—Co1—N6	92.22 (16)	C4—C3—H3D	110.5
N3—Co1—N6	173.73 (16)	H3C—C3—H3D	108.6
N4—Co1—N1	92.14 (18)	N4—C4—C3	106.5 (4)
N5—Co1—N1	174.76 (16)	N4—C4—H4C	110.4
N2—Co1—N1	84.87 (17)	C3—C4—H4C	110.4
N3—Co1—N1	91.56 (16)	N4—C4—H4D	110.4
N6—Co1—N1	93.26 (16)	C3—C4—H4D	110.4
C7—O1—In1	116.6 (3)	H4C—C4—H4D	108.6
C8—O3—In1	118.2 (3)	N5—C5—C6	107.9 (4)
C9—O5—In1	117.0 (3)	N5—C5—H5C	110.1
C10—O7—In1	114.6 (3)	C6—C5—H5C	110.1
C11—O9—In1	116.8 (3)	N5—C5—H5D	110.1
C12—O11—In1	116.9 (3)	C6—C5—H5D	110.1
In1—O13—H13A	118.1	H5C—C5—H5D	108.4
In1—O13—H13B	132.1	N6—C6—C5	106.2 (4)
H13A—O13—H13B	104.0	N6—C6—H6C	110.5
C1—N1—Co1	109.3 (3)	C5—C6—H6C	110.5
C1—N1—H1A	109.8	N6—C6—H6D	110.5
Co1—N1—H1A	109.8	C5—C6—H6D	110.5
C1—N1—H1B	109.8	H6C—C6—H6D	108.7
Co1—N1—H1B	109.8	O2—C7—O1	124.7 (4)
H1A—N1—H1B	108.3	O2—C7—C8	119.9 (4)
C2—N2—Co1	110.4 (3)	O1—C7—C8	115.4 (4)
C2—N2—H2A	109.6	O4—C8—O3	126.7 (4)

Co1—N2—H2A	109.6	O4—C8—C7	117.8 (4)
C2—N2—H2B	109.6	O3—C8—C7	115.6 (4)
Co1—N2—H2B	109.6	O6—C9—O5	125.6 (4)
H2A—N2—H2B	108.1	O6—C9—C10	118.4 (4)
C3—N3—Co1	110.6 (3)	O5—C9—C10	116.0 (4)
C3—N3—H3A	109.5	O8—C10—O7	125.0 (4)
Co1—N3—H3A	109.5	O8—C10—C9	118.4 (4)
C3—N3—H3B	109.5	O7—C10—C9	116.5 (4)
Co1—N3—H3B	109.5	O10—C11—O9	125.9 (5)
H3A—N3—H3B	108.1	O10—C11—C12	118.6 (4)
C4—N4—Co1	110.6 (3)	O9—C11—C12	115.5 (4)
C4—N4—H4A	109.5	O12—C12—O11	123.6 (5)
Co1—N4—H4A	109.5	O12—C12—C11	119.6 (4)
C4—N4—H4B	109.5	O11—C12—C11	116.8 (4)
Co1—N4—H4B	109.5		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O13—H13A···O12 ⁱ	0.91	1.79	2.620 (5)	150
O13—H13B···O6 ⁱⁱ	0.86	1.84	2.629 (4)	152
N1—H1A···O11 ⁱⁱⁱ	0.90	2.17	3.064 (5)	171
N1—H1B···O8 ^{iv}	0.90	2.14	2.972 (5)	153
N2—H2A···O7 ^v	0.90	2.10	2.935 (5)	155
N2—H2B···O10 ^{vi}	0.90	2.01	2.838 (5)	152
N3—H3A···O7 ^v	0.90	2.34	3.142 (5)	149
N3—H3A···O3 ^v	0.90	2.37	3.063 (5)	134
N3—H3B···O6 ^{iv}	0.90	2.06	2.878 (5)	151
N4—H4A···O1 ⁱⁱⁱ	0.90	2.26	3.114 (5)	159
N4—H4A···O2 ⁱⁱⁱ	0.90	2.49	3.103 (5)	126
N4—H4B···O2	0.90	2.04	2.924 (6)	168
N5—H5A···O8 ^v	0.90	2.09	2.962 (5)	163
N5—H5B···O4	0.90	2.14	2.912 (5)	143
N5—H5B···O2	0.90	2.40	3.099 (5)	135
N6—H6A···O11 ⁱⁱⁱ	0.90	2.27	3.040 (5)	143
N6—H6A···O1 ⁱⁱⁱ	0.90	2.49	3.279 (5)	147
N6—H6B···O10 ^{vi}	0.90	2.31	3.105 (5)	147

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+1, y, z$; (iii) $-x, -y+1, -z+2$; (iv) $-x, -y, -z+2$; (v) $-x+1, -y, -z+2$; (vi) $x, y, z+1$.

supplementary materials

Fig. 1

